REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-00-

0464

Public reporting burden for this collection of information is estimated to average 1 hour per response, incl ... ources, gathering and maintaining the data needed, and completing and reviewing the collection of information. ... of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Ser ... fferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Pa

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED 1 May 97 - 30 April 98

4. TITLE AND SUBTITLE Acquisition of a Computation/Visualization Server for the Center for Modeling and Simulation in Materials Science	5. FUNDING NUMBERS F49620-97-1-0305
6. AUTHOR(S) Diana Farkas	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Materials Science and Engineering Virginia Ploytechnic Institute & State University 213 Holden Hall, M/C 02371 Blacksburg, VA 24061	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR 801 N. Randolph Street, Room 732 Arlington, VA 22203-1977	10. SPONSORING/MONITORING AGENCY REPORT NUMBER F49620-99-1-0305
11. SUPPLEMENTARY NOTES	
12a. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release, unlimited distribution.	12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The computation/visualization server for the Center for Modeling and Simulation in Matehals Science (CMSMS) will support extensive computational research in fundamental areas of materials science that have an impact on the development and processing of novel matehals. DOD-supported research to be enhanced by the server will address the design and performance of novel matehals from first principles quantum mechanical calculations and non-equilibrium thermodynamic theories through the microslructural scale and up to the macroscopic level. Specifically, the research uses numerical simulation methods to investigate (i) the influence of crystal structure, defects, phase evolution, and interfaces on material properties, (ii) the mechanical properties ofpolycrystalline and fiber composites including the stochastic geometry and constituent material properties, (iii) the failure mode transition in the dynamic fracture of steels and (iv) the penetration of depleted uranium and tungsten heavy alloys into steel targets.

14. SUBJECT TERMS			15. NUMBER OF PAGES 7
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

Final Report on AFOSR 49620-97-1-0305

Title: Acquisition of a Computation/Visualization Server for the Center for Modeling and Simulation in Materials Science

Co-PIs: Diana Farkas, Romesh Batra, William Curtin, Ronald D. Kriz
Virginia Polytechnic Institute and State University, Blacksburg, Virginia

Amount: \$119,911 + \$30,000 Cost Sharing

Equipment Acquired:

Main Grant
3 Origin 2000 servers and 2 Octane workstations \$114,786.75
Supplemental memory \$3,670.00
Software \$311.50 Total \$118,768.25
The grant was underspent by \$1,142.75

Va Tech cost sharing
Supplemental memory \$16,183.00
Software \$3,320.00
Installation Supplies \$1,859.74
(3) Printers \$7,109.71
PC \$2,134.00
Total cost sharing \$30,606.45
Cost sharing required as per proposal = \$30,000

Use of the Equipment

The combination of server and workstations purchased served as the main server for CMSMS, the Center for Modeling and simulation in Materials Science. It supported extensive computational research in fundamental areas of materials science that have an impact on the development and processing of novel materials. The research addressed the design and performance of novel materials from first principles quantum mechanical calculations and non-equilibrium thermodynamic theories through the micro-structural scale and up to the macroscopic level. Numerical simulation methods were used to investigate:

(i) the influence of crystal structure, defects, phase evolution, and interfaces, on material properties (funded by ONR),

(ii) the mechanical properties of polycrystalline and fiber composites including the stochastic geometry and constituent material properties (funded by AFOSR),

(iii) the failure mode transitions in the dynamic fracture of steels (funded by ONR) and

(iv) the penetration of depleted uranium and tungsten heavy alloys into steel targets (funded by ARO).

The work accomplished by each Co-PI is listed below.

a) Professor Diana Farkas

A key component of the research work was the application of visualization techniques at all length scales from dislocation cores to shear bands. The equipment was used to perform the atomistic simulations and postprocess the enormous data sets generated, and complement the use of the virtual reality CAVE facility at Virginia Tech.

The visualization efforts were very important in the analysis of the physical phenomena studied in the simulations. The reseach also had an impact on the graduate edcational programs at Virginia Tech in the area of Mechanics and Materials.

The key resulting publications are listed below:

1) Ye F, Farkas D, Soboyejo W. : An investigation of fracture and fatigue crack growth behavior of cast niobium aluminide intermetallics, MAT SCI ENG A-STRUCT 264: (1-2) 81-93 MAY 31 1999

2) Vailhe C, Farkas D Transition from dislocation core spreading to dislocation dissociation in a series of B2 compounds PHILOS MAG A 79: (4) 921-931 APR 1999

3) Caillard D, Vailhe C, Farkas D: In-situ straining experiments in NiAl along soft orientations, and comparison with atomistic simulations PHILOS MAG A 79: (3) 723-739 MAR 1999

4) Mishin Y, Farkas D, Mehl MJ, et al. : Interatomic potentials for monoatomic metals from experimental data and ab initio calculations PHYS REV B 59: (5) 3393-3407 FEB 1 1999

5) Weertman JR, Farkas D, Hemker K, et al. Structure and mechanical behavior of bulk nanocrystalline materials MRS BULL 24: (2) 44-50 FEB 1999

6) Vailhe C, Farkas D: Interatomic potentials and dislocation simulation for the ternary B2 Ni-35Al-12Fe alloy MAT SCI ENG A-STRUCT 258: (1-2) 26-31 DEC 31 1998

7) Mutasa B, Farkas D: Effect of ordering energy and stoichiometry in Sigma=5 boundaries in B2 compounds METALL MATER TRANS A 29: (11) 2655-2668 NOV 1998

8) Mutasa B, Farkas D.: Atomistic structure of high-index surfaces in metals and alloys SURF SCI 415: (3) 312-319 OCT 9 1998

9) Farkas D :Fracture toughness from atomistic simulations: Brittleness induced by emission of sessile dislocations SCRIPTA MATER 39: (4-5) 533-536 AUG 4 1998

10) Mishin Y, Farkas D : Atomistic simulation of point defects end diffusion in B2 NiAl SCRIPTA MATER 39: (4-5) 625-630 AUG 4 1998

11) Farkas D: Atomistic simulations of fracture in the B2 phase of the Nb-Ti-Al system: MAT SCI ENG A-STRUCT 249: (1-2) 249-258 JUN 30 1998

12) Panova J, Farkas D: Atomistic simulation of dislocation core configurations in TiAl: PHILOS MAG A 78: (2) 389-404 AUG 1998

13) Farkas D, Cardozo FA: The multiplicity of possible grain boundary structures in Ni3Al INTERMETALLICS 6: (4) 257-268 JUN 1998

14) Mishin Y, Farkas D: Atomistic simulation of [001] symmetrical tilt grain boundaries in NiAl PHILOS MAG A 78: (1) 29-56 JUL 1998

Significant invited papers/presentaions/articles featuring our work

1) Weertman JR, Farkas D, Hemker K, et al. Structure and mechanical behavior of bulk nanocrystalline materials MRS BULL 24: (2) 44-50 FEB 1999

2) "A New view on Atoms" Interview with D. Farkas by Karen Green, ACCESS Magazine, 18, Fall/Winter 1998. National Center for Supercomputer Applications

3) Invited talk, Symposium on Fracture, Materials Research Society 1988 Fall meeting.

4) Press Conference, advances in Fracture, Materials Research Society 1998 Fall meeting.

5) Invited Talk, Lakeview Conference on Computational Materials Science, May 1998.

b) Professor R. C. Batra

The PI, five of his doctoral students and two masters students have been using the servers in their research. One doctoral student and one masters student completed all requirements for their degrees; the titles of their theses are listed below.
R. Gummalla, M.S., 1998, "Effect of Material and Geometric Parameters on Deformations of a Dynamically Loaded Prenotched plate".
S. S. Vel, Ph.D., 1998, "Analytical Solutions for the Deformation of Anisotropic Elastic and Piezothermoelastic Laminated Plates".

The Origin servers acquired with this grant were extensively used to study the failure mode transitions in a dynamically loaded prenotched plate. At low speeds of impact, brittle failure due to the maximum principal stress exceeding the limiting value ensues at a point on the upper surface of the notch tip. However, at high speeds of impact, a shear band initiates from a point on the lower surface of the notch tip and propagates into the plate. This failure mode transition is opposite to that observed in the Charpy V-notch test wherein a ductile failure ensues at low loading rates or at high temperatures and brittle failure at high loading rates or at low temperatures. We have computed the failure mode transition speed with four thermoviscoplastic relations, namely, the Litonski-Batra, Bodner-Partom, Johnson-Cook and the power law. Each one of these relations was calibrated with the same test data by solving initial-bounday-value problems closely simulating the test conditions. The failure mode transition speed found with these four relations is different.

The computing resources were also used to find the analytical solutions for thick elastic laminates under different boundary conditions. The analytical solution obtained by using the Eshelby-Stroh formalism is in the form of an infinite series and some of the coefficients are to be obtained by solving several small size eigen-value problems. The evaluation of displacements and stresses in different laminae is computationally intensive and could not have been carried out without the availability of these computing machines. The results exhibit boundary layer effects near the top and bottom surfaces of the laminate where loads are applied and also near the clamped and free edges.

The research results are described in the following publications and presentations.

Publications

1) R. C. Batra and R. R. Gummalla, Effect of Material and Geometric Parameters on Deformations Near the Notch-tip of a Dynamically Loaded Prenotched Plate, *Int. J. Fracture*, **101**, 99-140, 2000.

2) S. S. Vel and R. C. Batra, The Generalized Plane Strain Deformations of Thick Anisotropic Composite Laminated Plates, *Int. J. Solids Structures*, **37**, 715-733, 2000.

3) S. S. Vel and R. C. Batra, Cylindrical Bending of Laminated Plates with Distributed and Segmented Piezoelectric Actuator/Sensors, *AIAA J.*, **38**, 857-867, 2000.

4) S. Vel and R. C. Batra, Analytical Solutions for Rectangular Thick Laminated Plates Subjected to Arbitrary Boundary Conditions, *AIAA J.*, **37**, 1464-1473, 1999.

5) R. C. Batra and M. V. S. Ravisankar, Three-dimensional Numerical Simulation of the Kalthoff Experiment, *Int. J. Fracture* (in press).

6) S. S. Vel and R. C. Batra, Three-dimensional Analytical Solutions for Hybrid Multilayered Piezoelectric Plates, *J. Appl. Mechs.* (in press).

7) S. S. Vel and R. C. Batra, Generalized Plane Strain Thermoelastic Deformation of Laminated Anisotropic Thick Plates, *Int. J. Solids Structures* (in press).

8) R. C. Batra and L. Chen, Effect of Viscoplastic Relations on the Instability Strain, Shear Band Initiation Strain, the Strain Corresponding to the Minimum Shear Band Spacing, and the Band Width in a Thermoviscoplastic Materials, *Int. J. Plasticity* (accepted).

Presentations

1) R. D. Kriz, D. Farkas and R. C. Batra, Integrating Simulation Research into Curriculum Modules on Mechanical Behavior of Materials: From the Atomistic to the Continuum, *Materials Research Society Education Workshop*, Boston, Nov. 1998.

2) A. C. Loos, R. C. Batra, D. Rattazzi and A. Caba, A Three-Dimensional Simulation Model of the Resin Film Infusion Manufacturing Process, *30th Int. SAMPE Tech. Conf.*, San Antonio, TX, Oct. 1998.

3) R. C. Batra and L. Chen, Adiabataic Shear Band Spacing in Twelve Thermoviscoplastic Materials, *VI Pan American Congress of Applied Mechanics*, Rio de Janeiro, Brazil, Jan. 1999.

4) R. C. Batra and R. R. Gummalla, Analysis of Failure Modes in an Impact Loaded Prenotched Plate, *15th U.S. Army Symposium on Solid Mechanics*, Myrtle Beach, April 1999.

5) R. C. Batra, Effect of Material Parameterse and Constitutive Laws on the Failure Mode Transition in a Prenotched Steel Plate, *ONR Review*, Bethasda, MD, April 1999.

6) S. S. Vel and R. C. Batra, Analytical Solutions for the Deformation of Rectangular Plates Subjected to Arbitrary Boundary Conditions, *The 1999 ASME Mechanics & Materials Conf.*, Blacksburg, June 1999.

7) S. S. Vel and R. C. Batra, Analytical Solution for the Generalized Plane State of Deformation of Piezothermoelastic Laminated Plates, *The 1999 ASME Mechanics & Materials Conf.*, Blacksburg, June 1999.

8) R. C. Batra and L. Chen, Effect of Viscoplastic Relations on the Instability Strain, Shear Band Initiation Strain, the Strain Corresponding to the Minimum Shear Band Spacing, and the Band Width in a Thermoviscoplastic Material, *The 1999 ASME Mechanics & Materials Conf.*, Blacksburg, June 1999.

9) R. C. Batra, Analysis of Adiabatic Shear Bands with Four Viscoplastic Relations, ONR 6.1/6.2 Coordination Workshop, Bethasda, MD, May 2000.

10) R. C. Batra, Strain Localization in High Strain Rate Problems, (Invited lecture), *4th European Conf. on Solid Mechanics*, Metz, France, June 2000.

c) Professor William Curtin

The CMSMS Computational Facility was used extensively for computational modeling of the failure of fiber reinforced composites by Curtin and coworkers. In such composites, the stochastic fibers must be explicitly modeled and the composite deformation and tensile failure are intrinsically size-dependent. Useful numerical studies therefore consist of results on a sufficiently large composite (large number of fibers) and for large number of simulated realizations of the composite microstructure, so that appropriate size-scaling of the strength can be derived. In the period 1997-1998, we made extensive use of the CMSMS facility, as detailed below.

We primarily addressed the failure of Titanium matrix composites (TMCs) under a variety of "microstructures" (fiber geometries) and loading conditions. We first employed our existing composite model based on a Green's function technique to directly simulate the tensile strength of small specimens and compared directly to experimental results. With no adjustable parameters, the simulated composite strengths were found to be in excellent agreement with experiment for a range of fiber volume fractions, in-situ fiber strengths, and fiber/matrix interfacial sliding stresses. We then analyzed the influence of free boundaries on composite failure, as opposed to the commonly-used periodic boundary conditions. Broken fibers near a free surface or corner give higher stress concentrations on the neighboring fibers, and so can potentially drive composite failure at lower applied loads. Generating free surface boundary conditions to perform this study was accomplished using a method that was computationally very intensive and could not have been done without the new facility. Our results showed that free surfaces actually have a very minimal effect on composite strength. Using the same approach for obtaining free boundaries, we were then able to simulate the failure of TMCs under bending loads (not possible with periodic boundary conditions). This effort, again computationally very intensive, demonstrated how the damage in thin multiply TMCs propagates from ply to ply through the thickness in a stable manner. The simulations predicted the nominal bend strength of 6-ply TMCs in good agreement with experiments, whereas predictions using continuum models of the fiber deformation were much less accurate. Subsequently, we addressed the issue of non-uniform spatial distributions of the fibers in a TMC. The non-uniformity was accomplished starting from a regular array of fibers and removing fibers at random to create a "diluted" structure with a wide range of local fiber neighborhoods. The strengths of the "random" fiber arrangements were then compared to those of perfectly ordered fiber arrangements with the same spatial density of fibers. The simulations, in both cases, were again computationally demanding due to the method used to remove unwanted fibers. The results demonstrated that spatial disorder also has a very weak influence on composite strength. Such results could be rationalized through observation of the resulting critical damage states in the composites, which showed that significant local damage is necessary to drive failure. The precise local arrangement of the fibers (including the proximity of free boundaries) has a minor influence on the ultimate failure since damage must form over a larger scale. These conclusions were consistent with our analytic ideas on the nature of failure in these composite systems.

Publications:

1) G. C. Foster, M. Ibnabdeljalil, and W. A. Curtin, "Tensile Strength of Ti-MMCs: Direct Numerical Simulation and Analytic Models", Intl. J. Solids and Structures 35, 2523-2536 (1998).

2) G. C. Foster, MS Thesis, ESM Department, Virginia Polytechnic Institute and State University, Blacksburg, VA (1998).

3) W. A. Curtin, "Size Scaling of Strength in Fiber Composites", Physical Review Letters 80, 1445-1448 (1998).

4) W. A. Curtin and N. Takeda, "Tensile Strength of Fiber-reinforced Composites: I. Model and Effects of Local Fiber Geometry", J. Comp. Matls. 32, 2042-2059 (1998).

5) W. A. Curtin and N. Takeda, "Tensile Strength of Fiber-reinforced Composites: II. Application to Polymer Matrix Composites", J. Comp. Matls. 32, 2060-2081 (1998).

6) W. A. Curtin, B. K. Ahn, and N. Takeda, "Brittle and Tough Behavior in Ceramic Matrix Composites", Acta Mater. 3409-3420 (1998).

7) W. A. Curtin, B. K. Ahn, and N. Takeda, "Stress-strain behavior in CMCs: the Role of Interfacial Sliding", Ceramic Material Systems with Composite Structures, Ceramic Transactions (1998).

8) W. A. Curtin, "Stochastic Damage Evolution and Failure in Fiber-reinforced Composites", Advances in Applied Mechanics 36, 163-253 (1999).

d) Professor Ronald D. Kriz

The SGI mxi Octane workstations that was purchased with funds from the AFOSR project was particulary well suited for visual interpretation and analysis of supercomputer simulation results. Specifically this workstation was taken to the NSF Supercomputing at the University of Illinois, summer of 1997, where we developed the software application called "AtomView" Ref [1]. With AtomView material researchers could visually interpret and analyze nanostructures in three-dimensions. First on the SGI Octance workstation and when necessary in a fully immersive virtual environment of a CAVE(tm). This was done in collaboration with NCSA staff. All development was done on the SGI Octane workstation. AtomView was used in the development of curriculum modules for the Combined Research and Curriculum Development project, see Ref [2,3,4].

We continued to develope AtomView into a collaborative tool, see the CAVE Collaborative Console and AtomView (CCC-atom), Ref[5]. With CCC-atom researchers can now collaboratively interpret and analyze atomic structures simulated on supercomputers. Again this collaboration extends to fully immersive 3D virtual environments as well as the SGI Octane workstation. CCC-atom was entirely developed on the SGI Octane workstation purchased with AFOSR project funds.

References:

1) NCSA Access Article, "A New View of Atoms", http://access.ncsa.uiuc.edu/CoverStories/NewViewAtoms/atom.html

2) Kriz, R.D., Farkas, D., Batra, R.C., "Using Materials Resources on the World Wide Web for Introductory Materials Science Teaching," J. Materials Education, Vol. 19 no. (1&2), pp. 111-119, 1997.

3) Kriz, R.D., Farkas, D., Batra, R.C., "Integrating Simulation Research Into Curriculum Module on Mechanical Behavior of Materials: From the Atomistic to the Continuum," Presented at the MRS 1998 Workshop, J. Materials Education, Vol. 21, No. (1&2), pp. 43-52, 1999.

4) Kriz, R.D., Levensalor, R., Parikh, S., "Combined Research and Curriculum Development of Web and Java Based Educational Modules with Immersive Virtual Environments," Kluwer Academic Publishers, Conference Proceedings of the International Conference on Building University Electronic Educational Environments, University of California Irvine, August 4-6, 1999.

5) Web home page for CCC-atom: http://www.sv.vt.edu/future/cave/software/cccatom/

6) Invited talk, NRL Physical Metallurgy Branch, December 1998. Scientific visualization/ Materials Education (R. Kriz)